

# [1-bromo-2-methylpropane c4h9br structure](https://assignbuster.com/1-bromo-2-methylpropane-c4h9br-structure/)

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* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | C 4 H 9 Br  |
| Average mass  | 137. 018 Da  |
| Density  | 1. 3±0. 1 g/cm 3  |
| Boiling Point  | 90. 7±8. 0 °C at 760 mmHg  |
| Flash Point  | 18. 3±0. 0 °C  |
| Molar Refractivity  | 28. 3±0. 3 cm 3  |
| Polarizability  | 11. 2±0. 5 10 -24 cm 3  |
| Surface Tension  | 24. 6±3. 0 dyne/cm  |
| Molar Volume  | 108. 1±3. 0 cm 3  |

* Experimental data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Predicted – Mcule
* Experimental Physico-chemical Properties

## Experimental Melting Point:

|  |
| --- |
| -118 °CAlfa Aesar  |
| -118 °CJean-Claude Bradley Open Melting Point Dataset303  |
| -117 °CJean-Claude Bradley Open Melting Point Dataset13748  |
| -119 °CJean-Claude Bradley Open Melting Point Dataset21186  |
| -118 °CAlfa AesarB23854  |
| -117. 4 °CBiosynthJ-504405  |
| -119 °CLabNetworkLN00224680  |

## Experimental Boiling Point:

|  |
| --- |
| 90-92 °CAlfa Aesar  |
| 90-92 °CAlfa AesarB23854  |
| 90. 7 °CBiosynthJ-504405  |
| 90-92 °CLabNetworkLN00224680  |

## Experimental Flash Point:

|  |
| --- |
| 18 °CAlfa Aesar  |
| 18 °CAlfa Aesar  |
| 18 °F (-7. 7778 °C)Alfa AesarB23854  |
| 18 °CLabNetworkLN00224680  |

## Experimental Gravity:

|  |
| --- |
| 20 g/mLMerck Millipore1259  |
| 20 g/lMerck Millipore1259, 801549  |
| 1. 255 g/mLAlfa AesarB23854  |
| 18. 3 g/mLBiosynthJ-504405  |

## Experimental Refraction Index:

|  |
| --- |
| 1. 435Alfa AesarB23854  |

## Experimental Solubility:

|  |
| --- |
| -2. 43Egon Willighagenhttp://dx. doi. org/10. 1021/ci050282s  |
| Slightly soluble in water. Miscible with alcohol, etherAlfa AesarB23854  |

* Miscellaneous

## Safety:

|  |
| --- |
| 11-36/37/38Alfa AesarB23854  |
| 3Alfa AesarB23854  |
| 7-26-33-37-43Alfa AesarB23854  |
| DangerAlfa AesarB23854  |
| DANGER: FLAMMABLE, irritates skin, eyes, lungsAlfa AesarB23854  |
| H225-H315-H319-H335Alfa AesarB23854  |
| P210-P261-P303+P361+P353-P305+P351+P338-P405-P501aAlfa AesarB23854  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 651 (estimated with error: 62)NIST Spectramainlib\_227727, replib\_21078, replib\_58847, replib\_163852  |
| 666 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 ft; Column type: Packed; Start T: 27 C; CAS no: 78773; Active phase: Squalane; Carrier gas: He; Substrate: Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E., Variation of the retention index with temperature on squalane substrates, J. Gas Chromatogr., 6, 1968, 203-217.)NIST Spectranist ri  |
| 671 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 ft; Column type: Packed; Start T: 49 C; CAS no: 78773; Active phase: Squalane; Carrier gas: He; Substrate: Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E., Variation of the retention index with temperature on squalane substrates, J. Gas Chromatogr., 6, 1968, 203-217.)NIST Spectranist ri  |
| 676 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 ft; Column type: Packed; Start T: 67 C; CAS no: 78773; Active phase: Squalane; Carrier gas: He; Substrate: Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E., Variation of the retention index with temperature on squalane substrates, J. Gas Chromatogr., 6, 1968, 203-217., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 1. 5 m; Column type: Packed; Start T: 78 C; CAS no: 78773; Active phase: Squalane; Carrier gas: Mixture; Substrate: Celite; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 1. 8 m; Column type: Packed; Start T: 78 C; CAS no: 78773; Active phase: Squalane; Carrier gas: N2; Substrate: Celite; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302.)NIST Spectranist ri  |
| 680 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 ft; Column type: Packed; Start T: 86 C; CAS no: 78773; Active phase: Squalane; Carrier gas: He; Substrate: Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E., Variation of the retention index with temperature on squalane substrates, J. Gas Chromatogr., 6, 1968, 203-217., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 1. 5 m; Column type: Packed; Start T: 100 C; CAS no: 78773; Active phase: Squalane; Carrier gas: Ar; Substrate: Celite; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302.)NIST Spectranist ri  |
| 672 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 1. 5 m; Column type: Packed; Start T: 65 C; CAS no: 78773; Active phase: Squalane; Carrier gas: Ar; Substrate: Celite; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302.)NIST Spectranist ri  |
| 673 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 1. 5 m; Column type: Packed; Start T: 65 C; CAS no: 78773; Active phase: Squalane; Carrier gas: Mixture; Substrate: Celite; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 1. 8 m; Column type: Packed; Start T: 65 C; CAS no: 78773; Active phase: Squalane; Carrier gas: N2; Substrate: Celite; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302.)NIST Spectranist ri  |
| 674 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 1. 2 m; Column type: Packed; Start T: 65 C; CAS no: 78773; Active phase: Squalane; Carrier gas: Ar; Substrate: Celite; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 65 C; CAS no: 78773; Active phase: Squalane; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302.)NIST Spectranist ri  |
| 675 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 1. 5 m; Column type: Packed; Start T: 78 C; CAS no: 78773; Active phase: Squalane; Carrier gas: Ar; Substrate: Celite; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302.)NIST Spectranist ri  |
| 677 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 0. 9 m; Column type: Packed; Start T: 65 C; CAS no: 78773; Active phase: Squalane; Carrier gas: He; Substrate: Celite; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 1. 2 m; Column type: Packed; Start T: 78 C; CAS no: 78773; Active phase: Squalane; Carrier gas: Ar; Substrate: Celite; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 78 C; CAS no: 78773; Active phase: Squalane; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302.)NIST Spectranist ri  |
| 679 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 0. 9 m; Column type: Packed; Start T: 78 C; CAS no: 78773; Active phase: Squalane; Carrier gas: He; Substrate: Celite; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 1. 5 m; Column type: Packed; Start T: 100 C; CAS no: 78773; Active phase: Squalane; Carrier gas: Mixture; Substrate: Celite; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302.)NIST Spectranist ri  |
| 681 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 1. 8 m; Column type: Packed; Start T: 100 C; CAS no: 78773; Active phase: Squalane; Carrier gas: N2; Substrate: Celite; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302.)NIST Spectranist ri  |
| 682 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 100 C; CAS no: 78773; Active phase: Squalane; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302.)NIST Spectranist ri  |
| 686 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 0. 9 m; Column type: Packed; Start T: 100 C; CAS no: 78773; Active phase: Squalane; Carrier gas: He; Substrate: Celite; Data type: Kovats RI; Authors: Adlard, E. R.; Evans, M. B.; Butlin, A. G.; Evans, R. S.; Hill, R.; Huber, J. F. K.; Littlewood, A. B.; McCambley, W. G.; Smith, J. F.; Swanton, W. T.; Swoboda, P. A. T., Recommendations of the data sub-committee for the publication of retention data, J. Gas Chromatogr., , 1965, 298-302.)NIST Spectranist ri  |
| 699 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 70 C; CAS no: 78773; Active phase: Apiezon L; Substrate: Celite (40: 60 Gewichtsverhaltnis); Data type: Kovats RI; Authors: von Kovats, E., 206. Gas-chromatographische Charakterisierung organischer Verbindungen. Teil 1: Retentionsindices aliphatischer Halogenide, Alkohole, Aldehyde und Ketone, Helv. Chim. Acta, 41(7), 1958, 1915-1932.)NIST Spectranist ri  |
| 711 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 130 C; CAS no: 78773; Active phase: Apiezon L; Substrate: Celite (40: 60 Gewichtsverhaltnis); Data type: Kovats RI; Authors: von Kovats, E., 206. Gas-chromatographische Charakterisierung organischer Verbindungen. Teil 1: Retentionsindices aliphatischer Halogenide, Alkohole, Aldehyde und Ketone, Helv. Chim. Acta, 41(7), 1958, 1915-1932.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 677 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 78773; Active phase: Methyl Silicone; Data type: Normal alkane RI; Authors: Zenkevich, I. G.; Marinichev, A. N., Comparison of Topological and Dynamics Molecular Characteristics for Precalculation of Chromatographic Retention Parameters of Organic Compounds (in Russian), Zh. Struct. Khim., 42(5), 2001, 893-902, In original 893-902.)NIST Spectranist ri  |
| 677. 2 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; CAS no: 78773; Active phase: Silicone oil; Carrier gas: N2; Data type: Normal alkane RI; Authors: Hepburn, D. R.; Hudson, H. R., Gas chromatography of alkyl halides on a silicone oil capillary column, J. Chromatogr., 103, 1975, 166-169.)NIST Spectranist ri  |

Predicted data is generated using the ACD/Labs Percepta Platform – PhysChem Module

|  |  |
| --- | --- |
| Density:  | 1. 3±0. 1 g/cm 3  |
| Boiling Point:  | 90. 7±8. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 62. 9±0. 2 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 31. 3±0. 0 kJ/mol  |
| Flash Point:  | 18. 3±0. 0 °C  |
| Index of Refraction:  | 1. 436  |
| Molar Refractivity:  | 28. 3±0. 3 cm 3  |
| #H bond acceptors:  | 0  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 1  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 2. 56  |
| ACD/LogD (pH 5. 5):  | 2. 46  |
| ACD/BCF (pH 5. 5):  | 43. 32  |
| ACD/KOC (pH 5. 5):  | 516. 61  |
| ACD/LogD (pH 7. 4):  | 2. 46  |
| ACD/BCF (pH 7. 4):  | 43. 32  |
| ACD/KOC (pH 7. 4):  | 516. 61  |
| Polar Surface Area:  | 0 Å 2  |
| Polarizability:  | 11. 2±0. 5 10 -24 cm 3  |
| Surface Tension:  | 24. 6±3. 0 dyne/cm  |
| Molar Volume:  | 108. 1±3. 0 cm 3  |

Predicted data is generated using the US Environmental Protection Agency’s EPISuite™

 Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 2. 58Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 87. 38 (Adapted Stein & Brown method)Melting Pt (deg C): -78. 08 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 62 (Mean VP of Antoine & Grain methods)MP (exp database): -119 deg CBP (exp database): 91. 1 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 543. 9log Kow used: 2. 58 (estimated)no-melting pt equation usedWater Sol (Exper. database match) = 507 mg/L (18 deg C)Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1285. 6 mg/LWat Sol (Exper. database match) = 507. 00Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 99E-002 atm-m3/moleGroup Method: 1. 94E-002 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 2. 055E-002 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 58 (KowWin est)Log Kaw used: -0. 090 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 2. 670Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6361Biowin2 (Non-Linear Model) : 0. 0329Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 9253 (weeks )Biowin4 (Primary Survey Model) : 3. 6854 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4008Biowin6 (MITI Non-Linear Model): 0. 1656Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 8962Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 7. 93E+003 Pa (59. 5 mm Hg)Log Koa (Koawin est ): 2. 670Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 78E-010 Octanol/air (Koa) model: 1. 15E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 37E-008 Mackay model : 3. 03E-008 Octanol/air (Koa) model: 9. 19E-009 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 1. 5486 E-12 cm3/molecule-secHalf-Life = 6. 907 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 82. 881 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 2. 2E-008 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 67. 7Log Koc: 1. 831 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Total Kb for pH > 8 at 25 deg C : 1. 203E-010 L/mol-secKb Half-Life at pH 8: 1. 826E+008 years Kb Half-Life at pH 7: 1. 826E+009 years Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 1. 283 (BCF = 19. 2)log Kow used: 2. 58 (estimated)Volatilization from Water: Henry LC: 0. 0194 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 1. 23 hoursHalf-Life from Model Lake : 111. 6 hours (4. 649 days)Removal In Wastewater Treatment: Total removal: 88. 39 percentTotal biodegradation: 0. 03 percentTotal sludge adsorption: 1. 38 percentTotal to Air: 86. 98 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 41. 6 166 1000 Water 45. 6 360 1000 Soil 12. 4 720 1000 Sediment 0. 362 3. 24e+003 0 Persistence Time: 136 hr

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop